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AIR POLLUTION MODELING BY QUASILINEARIZATION

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Abstract—The quasilinearization technique which was developed by Dr. Bellman, has been shown to be an effective technique for solving the inverse problem in modeling. In this work this technique is applied to the modeling of the air pollution and diffusion problem. Numerical results are given to illustrate the effectiveness of the approach.

INTRODUCTION

The dispersion of air pollutants is a function of the emission source, topography, and meteorological factors. The complex influences of these factors make the modeling of air pollutants extremely difficult. To further complicate the situation, the various meteorological factors are unstable and are changing or fluctuating constantly. To represent these complicated phenomena, various statistical and deterministic approaches have been proposed [1–10]. Simulation and game theory have also been applied [3,4]. One common feature in the modeling of air pollution is the requirement of the estimation of the parameters.

Bellman named these estimation problems as the inverse problem, which is a basic and difficult problem in establishing any model. To overcome this difficulty, Bellman and coworkers [11,12] developed two effective techniques: quasilinearization and invariant imbedding. Invariant imbedding has been applied to air pollution control in an earlier paper [13]. Quasilinearization is applied to a simple air pollution problem to illustrate the approach in this work.

A SIMPLE AIR POLLUTION MODEL

To illustrate the approach, we shall consider a simple air pollution model. Obviously, the approach can be easily applied to much more complicated models.

Turbulent diffusion from an elevated point source is of primary concern in air pollution meteorology. But atmospheric diffusion has such an intricate mechanism that no model can satisfy all demands. One model, which is fairly general, can be represented by the following parabolic diffusion equation

$$u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}+\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left[K_x\frac{\partial C}{\partial x}\right]+\frac{\partial}{\partial y}\left[K_y\frac{\partial C}{\partial y}\right]+\frac{\partial}{\partial z}\left[K_z\frac{\partial C}{\partial z}\right], \tag{1}$$

where

C = average concentration,
x, y, z = space coordinates,
u, v, w = average wind components,
K_i = coefficient of eddy diffusivity in the i-direction,
t = time.

To simplify the model, we shall only consider steady state conditions, with wind speed and eddy diffusivity remaining constant over the region. A point source was considered. The model was arranged so that the origin was at the source, the x-axis oriented down wind, the y-axis cross wind and the z-axis vertical. According to these simplifying assumptions and using dimensionless variables, equation (1) becomes

$$\frac{\partial S}{\partial \bar{x}} = \frac{\partial^2 S}{\partial Y^2} + \frac{\partial^2 S}{\partial Z^2} - V\frac{\partial S}{\partial Y}, \tag{2}$$

where

$$\begin{aligned} S &= C/C_0, \quad \bar{x} = Kx/uH^2, \\ Y &= y/H, \quad V = Hv/K, \\ Z &= z/H. \end{aligned}$$

By applying finite differences, equation (2) can now be reduced into a set of ordinary differential equations

$$\begin{aligned} \frac{dS}{d\bar{x}}|_{m,n} = \frac{1}{\Delta Y(m)} &\left(\frac{S(m+1,n)-S(m,n)}{\Delta Y(m+\frac{1}{2})} \frac{S(m,n)-S(m-1,n)}{\Delta Y(m-\frac{1}{2})}\right) \\ &+ \frac{S(m,n+1)-2\,S(m,n)+S(m,n-1)}{\Delta Z^2} - V_n \frac{S(m+1,n)-S(m-1,n)}{2\,\Delta Y(m)}, \end{aligned} \tag{3}$$

where m and n are the grid sizes in the Y and Z directions, respectively.

The fairly simple model presented by Brock and Hewson [8] was used in this work. There are total of 25 cells in this model (see Figure 1). Equation (3) can now be rewritten as

$$\begin{aligned} \frac{dS}{dX}|_{m,n} = \frac{1}{25\,\Delta Y(m)} &\left(\frac{S(m+1,n)-S(m,n)}{\Delta Y(m+\frac{1}{2})} - \frac{S(m,n)-S(m-1,n)}{\Delta Y(m-\frac{1}{2})}\right) \\ &- \frac{V_n}{50\,\Delta Y(m)}[S(m+1,n)-S(m-1,n)] + [S(m,n+1)-2\,S(m,n)+S(m,n-1)], \end{aligned} \tag{4}$$

where $X = 25\,\bar{x}$ and the boundary conditions are:

$$\begin{aligned} S(-2,n) &= 0, & S(m,5) &= S(m,6), \\ S(2,n) &= 0, & S(0,3)|_0 &= 1, \\ S(m,0) &= S(m,1), \end{aligned}$$

with $m = 0,1,2$; $n = 1,2,\ldots,5$. Let $S(m,n)$ represent the concentration of cell (m,n) and also let

$$\begin{aligned} S(0,1) &= x1, & S(1,1) &= x6, & S(-1,1) &= x11, \\ S(0,2) &= x2, & S(1,2) &= x7, & S(-1,2) &= x12, \\ S(0,3) &= x3, & S(1,3) &= x8, & S(-1,3) &= x13, \\ S(0,4) &= x4, & S(1,4) &= x9, & S(-1,4) &= x14, \\ S(0,5) &= x5, & S(1,5) &= x10, & S(-1,5) &= x15. \end{aligned}$$

According to Figure 1, we have

$$\Delta Y(m) = 0.2\exp\left[\frac{0.917m}{(2-m)}\right],$$

$$\Delta Y(0.5) = 0.2\exp\left[0.917 \times \frac{0.5}{(2-0.5)}\right] = 0.2714,$$

$$\Delta Y(1.5) = 0.2\exp\left[0.917 \times \frac{1.5}{(2-1.5)}\right] = 3.12.$$

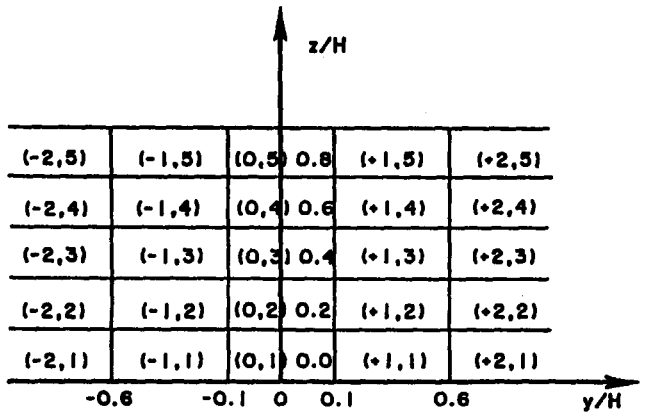

Figure 1. Schematic representation of a 25-cell model [8].

Let

$$A = \frac{0.2}{\Delta Y(0.5)} = 0.7369,$$
$$A6 = \frac{0.08}{\Delta Y(0.5)} = 0.2948,$$
$$B = \frac{0.08}{\Delta Y(1.5)} = 0.0256.$$

Substituting the above values into equation (4), we obtain 15 differential equations for the 15 cells. Notice that 10 boundary cells have been assumed zero in equation (4). These 15 equations are:

$$\frac{dS(0,1)}{dX} = \frac{dx1}{dX} = (A - 0.1\,V_1)\,x6 - 2.4738\,x1 + (A + 0.1\,V_1)\,x11 + x2, \tag{5}$$
$$\frac{dS(0,2)}{dX} = \frac{dx2}{dX} = (A - 0.1\,V_2)\,x7 - 3.4738\,x2 + (A + 0.1\,V_2)\,x12 + x3 + x1, \tag{6}$$
$$\frac{dS(0,3)}{dX} = \frac{dx3}{dX} = (A - 0.1\,V_3)\,x8 - 3.4738\,x3 + (A + 0.1\,V_3)\,x13 + x4 + x2, \tag{7}$$
$$\frac{dS(0,4)}{dX} = \frac{dx4}{dX} = (A - 0.1\,V_4)\,x9 - 2.4738\,x4 + (A + 0.1\,V_4)\,x14 + x5 + x3, \tag{8}$$
$$\frac{dS(0,5)}{dX} = \frac{dx5}{dX} = (A - 0.1\,V_5)\,x10 - 2.4738\,x5 + (A + 0.1\,V_5)\,x15 + x4, \tag{9}$$
$$\frac{dS(1,1)}{dX} = \frac{dx6}{dX} = -1.3204\,x6 + (A6 + 0.04\,V_1)\,x1 + x7, \tag{10}$$
$$\frac{dS(1,2)}{dX} = \frac{dx7}{dX} = -2.3204\,x7 + (A6 + 0.04\,V_2)\,x2 + x8 + x6, \tag{11}$$
$$\frac{dS(1,3)}{dX} = \frac{dx8}{dX} = -2.3204\,x8 + (A6 + 0.04\,V_3)\,x3 + x9 + x7, \tag{12}$$
$$\frac{dS(1,4)}{dX} = \frac{dx9}{dX} = -2.3204\,x9 + (A6 + 0.04\,V_4)\,x4 + x10 + x8, \tag{13}$$
$$\frac{dS(1,5)}{dX} = \frac{dx10}{dX} = -1.3204\,x10 + (A6 + 0.04\,V_5)\,x5 + x9, \tag{14}$$
$$\frac{dS(-1,1)}{dX} = \frac{dx11}{dX} = (A6 - 0.04\,V_1)\,x1 - 1.3204\,x11 + x12, \tag{15}$$
$$\frac{dS(-1,2)}{dX} = \frac{dx12}{dX} = (A6 - 0.04\,V_2)\,x2 - 2.3204\,x12 + x13 + x11, \tag{16}$$
$$\frac{dS(-1,3)}{dX} = \frac{dx13}{dX} = (A6 - 0.04\,V_3)\,x3 - 2.3204\,x13 + x14 + x12, \tag{17}$$

$$\frac{dS(-1,4)}{dX} = \frac{dx14}{dX} = (A6 - 0.04\,V_4)\,x4 - 2.3204\,x14 + x15 + x13, \tag{18}$$

$$\frac{dS(-1,5)}{dX} = \frac{dx15}{dX} = (A6 - 0.04\,V_5)\,x5 - 1.3204\,x15 + x14. \tag{19}$$

The given initial conditions are:

$$\begin{aligned} &xn(0) = 0, \qquad n = 1,2,4,5,\ldots,15, \\ &xn(0) = 1, \qquad n = 3. \end{aligned} \tag{20}$$

PARAMETER ESTIMATION

Consider equation (4), or the more detailed equations (5)–(19), in an actual experimental situation, the coefficients in these equations, such as V_n cannot be measured. Only the concentrations of different regions or cells can be measured at various downstream distances. Thus, V_n must be estimated from these measured data. This estimation problem becomes very difficult if closed form solutions for the equations cannot be found. Bellman's approach of using quasilinearization to solve this estimation problem directly from the original differential equations has been shown to be very effective. Furthermore, even if closed form solutions for the process model could be obtained, the quasilinearization approach of directly estimating the parameters from the differential equations still has distinct advantages. The parameters (or wind direction shear constants) appear nonlinearly in the resulting analytical solutions of equation (4). The estimation of parameters from nonlinear algebraic equations is not easy. The quasilinearization technique appears to be much more powerful than the commonly used nonlinear regression or nonlinear least squares estimation techniques.

The problem now can be stated as follows: Estimate the wind direction shear constants, V_n $(1,2,\ldots,5)$, for equation (4) with the following measured or experimental data

$$\begin{aligned} &x1^{(\exp)}(X_s) = x1_s, \qquad s = 1,2,\ldots,S, \\ &x2^{(\exp)}(X_r) = x2_r, \qquad r = 1,2,\ldots,R, \\ &\vdots \\ &x15^{(\exp)}(X_q) = x15_q, \qquad q = 1,2,\ldots,Q, \end{aligned}$$

with the required constraint

$$S + R + \ldots + Q \geq 5.$$

Obviously the more data the better, and the minimum number of data required has to be equal to the number of unknowns to be estimated, assuming the data are exactly correct and have no errors. The quantities $x1_s, x2_r, \ldots, x15_q$ are known values and are obtained by measuring the concentrations of pollutants at various values of X. The number of the experimental values must be greater than or equal to the number of the unknown constant parameters. The superscript, (exp), means that the values of $x1, x2, \ldots, x15$ are experimental values.

In order to estimate the five unknown parameters or the five wind shear constants V_i, $i = 1,2,\ldots,5$, we establish the five trivial differential equations.

$$\frac{dV_1}{dX} = 0, \tag{21}$$

$$\frac{dV_2}{dX} = 0, \tag{22}$$

$$\frac{dV_3}{dX} = 0, \tag{23}$$

$$\frac{dV_4}{dX} = 0, \tag{24}$$

$$\frac{dV_5}{dX} = 0. \tag{25}$$

Now, our system has twenty differential equations. Fifteen initial conditions are given in equation (20). The other five conditions can be obtained from the experimental data by using least squares.

THE LEAST SQUARE APPROACH

Since in practical situations the experimental data are seldom exact, and generally have experimental or measurement errors, it is therefore desirable to obtain many data points instead of just the minimum number. The classical least squares criterion can be used to take care of the extra data. The objective is to determine the constant parameters or coefficients so that the sum of the squares of the deviations is minimized, by using the following expression:

$$Q = \sum_{s=1}^{S}[x1(X_s) - x1_s]^2 + \sum_{r=1}^{R}[x2(X_r) - x2_r]^2 + \ldots + \sum_{q=1}^{Q}[x15(X_q) - x15_q]^2, \tag{26}$$

where the minimization is over the constant parameters, V_1, V_2, V_3, V_4 and V_5. The values of $x1(X_s), x2(X_r), \ldots, x15(X_q)$ are obtained by solving equations (5)–(19).

Thus, by minimizing equation (26) with respect to the five wind shear constants, five additional conditions can be obtained for the system of twenty equations.

QUASILINEARIZATION

The quasilinearization technique is well known. We shall not give a detailed description. Only the minimum essentials will be discussed here.

When the wind shear constants, V, are considered as unknown, equations (5)–(19) are nonlinear. Quasilinearization will be used to solve these twenty equations and, at the same time, to estimate the five unknown constants. By applying the following generalized Newton-Raphson formula, which is essentially the Taylor series expansion with second and higher order terms omitted, equations (5)–(19) can be linearized simultaneously

$$\frac{dX_{k+1}}{dt} = \underset{\sim}{f}(\underset{\sim}{X}_k, t) + \underset{\sim}{J}(\underset{\sim}{X}_k)(\underset{\sim}{X}_{k+1} - \underset{\sim}{X}_k). \tag{27}$$

The linearized equations are fairly lenghty. We shall not list all of them here. For example for equation (5), the linearized equation is:

$$\begin{aligned}\frac{dx1_{k+1}}{dX} = &- 2.4738\, x1_{k+1} + x2_{k+1} + (A - 0.1\, V_{1,k})\, x6_{k+1} + (A + 0.1\, V_{1,k})\, x11_{k+1} \\ &+ (A - 0.1\, V_{1,k})\, x6_{k+1} - (0.1\, x11_k - 0.1\, x6_k)\, V_{1,k}.\end{aligned} \tag{28}$$

These twenty linear equations can be solved together with the twenty conditions given by equations (20) and the least square minimization of equation (26). Since these equations are linear, they can be solved by the use of the superposition principle [12] iteratively.

COMPUTATIONAL PROCEDURE

The superposition principle for the solution of the linearized versions of equations (5)–(19) can be represented as follows:

$$\underset{\sim}{x}_{k+1}(X) = \underset{\sim}{x}_{p,k+1}(X) + \underset{\sim}{x}_{h,k+1}(X)\, \underset{\sim}{a}_{k+1}, \tag{29}$$

where $\underset{\sim}{x}_{k+1}(X)$ is the solution vector of the linearized equations, with $0 \leq X \leq X_f$.

The solution vector for the state $\underset{\sim}{x}_{k+1}(X)$ and the particular solution vector $x_{p,k+1}(X)$ are defined as

$$\underset{\sim}{x}_{k+1} = \begin{pmatrix} x1_{k+1}(X) \\ x2_{k+1}(X) \\ \vdots \\ x15_{k+1}(X) \end{pmatrix} \quad \text{and} \quad \underset{\sim}{x}_{p,k+1}(X) = \begin{pmatrix} x1_{p,k+1}(X) \\ x2_{p,k+1}(X) \\ \vdots \\ x15_{p,k+1}(X) \end{pmatrix}, \tag{30}$$

respectively. The integration constant vector is

$$\underset{\sim}{a}_{k+1} = \begin{pmatrix} a_{1,k+1} \\ a_{2,k+1} \\ a_{3,k+1} \\ a_{4,k+1} \\ a_{5,k+1} \end{pmatrix}. \tag{31}$$

The homogeneous solution matrix is defined by

$$\underset{\sim}{x}_{h,k+1}(X) = \begin{pmatrix} x1_{h1,k+1}(X) & x1_{h2,k+1}(X) & \dots & x1_{h5,k+1}(X) \\ x2_{h1,k+1}(X) & x2_{h2,k+1}(X) & \dots & x2_{h5,k+1}(X) \\ \vdots & \vdots & & \vdots \\ x15_{h1,k+1}(X) & x15_{h2,k+1}(X) & \dots & x15_{h5,k+1}(X) \end{pmatrix}. \tag{32}$$

The particular and homogeneous solutions were chosen in such a way that they satisfy the fifteen given initial conditions, equation (20). Thus, only five sets of homogeneous solutions and five integration constants were needed. In actual calculations, the set of particular solutions were obtained by integrating the linearized equation with the following initial values

$$\underset{\sim}{x}_{p,k+1}(0) = \begin{pmatrix} x1^0 \\ x2^0 \\ \vdots \\ x15^0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{33}$$

The initial values used for the five sets of homogeneous solutions were

$$\underset{\sim}{x}_{h,k+1}(0) = \begin{pmatrix} \underset{\sim}{A} \\ - - \\ \underset{\sim}{B} \end{pmatrix}, \tag{34}$$

where

$$\underset{\sim}{A} = \underset{\sim}{0},$$

$$\underset{\sim}{B} = \underset{\sim}{I}.$$

$\underset{\sim}{A}$ is a (15 × 5) zero matrix, and $\underset{\sim}{B}$ is a (5 × 5) identity matrix. Again, notice that the initial values in equations (33) and (34) were chosen in such a way that at $t = 0$, the general solutions of $x1, x2, \dots, x15$ in equation (29) satisfied the given initial conditions, equation (22). Thus, only five sets of homogeneous solutions were needed.

Fifteen initial conditions are given. The remaining five conditions can be obtained by minimizing equation (26). This minimization can be done either numerically or analytically. In this work, the analytical approach was used. Substitute equation (29) into equation (26) and then

differentiate the resulting equation with respect to $a_{j,k+1}$, $j = 1,2,\ldots 5$, we have

$$\begin{aligned}\frac{\partial Q_{k+1}}{\partial a_{i,k+1}} &= 2\sum_{s=1}^{S} x1_{hj,k+1}(X_s)\left[x1_{p,k+1}(X_s) + \sum_{j=1}^{5} a_{j,k+1}\, x1_{hj,k+1}(X_s) - x1_s\right] \\ &\quad + 2\sum_{r=1}^{R} x2_{hj,k+1}(X_r)\left[x2_{p,k+1}(X) + \sum_{j=1}^{5} a_{j,k+1}\, x2_{hj,k+1}(X_r) - x2_r\right] \\ &\quad \vdots \\ &\quad + 2\sum_{q=1}^{Q} x15_{hj,k+1}(X_q)\left[x15_{p,k+1}(X_q) + \sum_{j=1}^{5} a_{j,k+1}\, x15_{hj,k+1}(X_q) - x15_q\right] \\ &= 0, \qquad i = 1,2,3,4, \text{ and } 5.\end{aligned} \tag{35}$$

These five equations form the remaining five boundary conditions, the values of $a_{j,k+1}$, $j = 1,2,3,4,5$ can now be obtained by solving the above five algebraic equations. Once the integration constants are known, the general solutions for $x1_{k+1}(X), x2_{k+1}(X),\ldots, x15_{k+1}(X)$; $V_{1,k+1}(X), V_{2,k+1}(X),\ldots, V_{5,k+1}(X)$ can be obtained from equation (29).

With $x1_{k+1}, x2_{k+1},\ldots, x15_{k+1}$; $V_{1,k+1}, V_{2,k+1},\ldots, V_{5,k+1}$ known, an improved set of values can then be obtained in the same way, by making $k = k+1$ in the linearized equations such as equation (28). This iterative procedure is continued until the desired accuracy is obtained.

The computational procedure can now be summarized as follows:

1. Linearize the system of equations (5)–(19) and (21)–(25), using the generalized Newton-Raphson equation (27).
2. Assume a set of reasonable initial functions for $x1(X)$, $x2(X),\ldots, x15(X)$; $V_1(X)$, $V_2(X)$, $\ldots$, $V_5(X)$. Let these initial functions be $x1_{k=0}(X)$, $x2_{k=0}(X),\ldots, x15_{k=0}(X)$; $V_{1,k=0}(X)$, $V_{2,k=0}(X),\ldots, V_{5,k=0}(X)$.
3. Integrate the linearized equations numerically using (33) as the initial value with $k = 0$.
4. Integrate the homogeneous form of the linearized equations five times using (34) as the initial value with $k = 0$.
5. Solve equation (35) for the integration constants $a_{j,k+1=1}$, $j = 1,2,\ldots,5$, using the newly obtained particular and homogeneous solutions from Steps 3 and 4, and using the given experimental data, $x1_s$, $x2_r,\ldots, x15_q$ ($s = 1,2,\ldots,S$; $r = 1,2,\ldots,R$; $\ldots$; $p = 1,2,\ldots,P$; $q = 1,2,\ldots,Q$).
6. Calculate $x1_{k+1=1}$, $x2_{k+1=1}(X),\ldots, x15_{k+1=1}(X)$; $V_{1,k+1=1}(X)$, $V_{2,k+1=1}(X)$, $\ldots$, $V_{5,k+1=1}(X)$ using equations (29).
7. Repeat Steps 3 through 5 with $k = 1,2,\ldots$, until no further improvement on the values of $x1(X)$, $x2(X),\ldots, x15(X)$, V_1, $V_2,\ldots, V_5$ can be obtained.

Note that the best available initial functions should be used for Step 2.

NUMERICAL RESULTS

To illustrate the effectiveness of this approach, the constants in equations (5)–(19) were estimated. The data used were obtained numerically by solving equations (5)–(19) using the following values

$$\begin{aligned} x1(0) &= 0, & x2(0) &= 0, & x3(0) &= 1 \\ x4(0) &= 0, & x5(0) &= 0, & x6(0) &= 0 \\ x7(0) &= 0, & x8(0) &= 0, & x9(0) &= 0 \\ x10(0) &= 0, & x11(0) &= 0, & x12(0) &= 0 \\ x13(0) &= 0, & x14(0) &= 0, & x15(0) &= 0 \\ X_f &= 5, & V_2 &= 1.35, & V_4 &= -1.11 \\ V_1 &= 2.99, & V_3 &= 0, & V_5 &= -1.99. \end{aligned}$$

Equations (5)–(19) were integrated numerically with the Runge-Kutta integration scheme. The step size used was $\Delta X = 0.05$. The results were then corrupted with noise by the following equations.

$$x1Z^{(\exp)}(I) = x1S(I) + R_1,$$
$$x2Z^{(\exp)}(I) = x2S(I) + R_2,$$
$$\vdots \qquad\qquad \vdots$$
$$x15Z^{(\exp)}(I) = x15S(I) + R_{15},$$

where xZ represents the noisy data, xS represents the data before corrupted with noise and the Rs are normally distributed random numbers. The means for these random numbers were a zero.

The I represents the data points used. Since the integration step size used was 0.05 and the duration of the independent variable X, was 5, there are a total of 100 integration steps. In this work, we only used 11 data points. In other words, the results of every tenth integration step were used as data points. Thus, $I = 1, 2, 3, \ldots, 11$ correspond to integration grid points $1, 11, 21, \ldots, 101$, respectively.

Both 5% and 10% noisy data were used. Sample data for exact, 5% and 10% noise levels are shown in Figures 2, 3, and 4. Because of space, the complete data used will not be listed here.

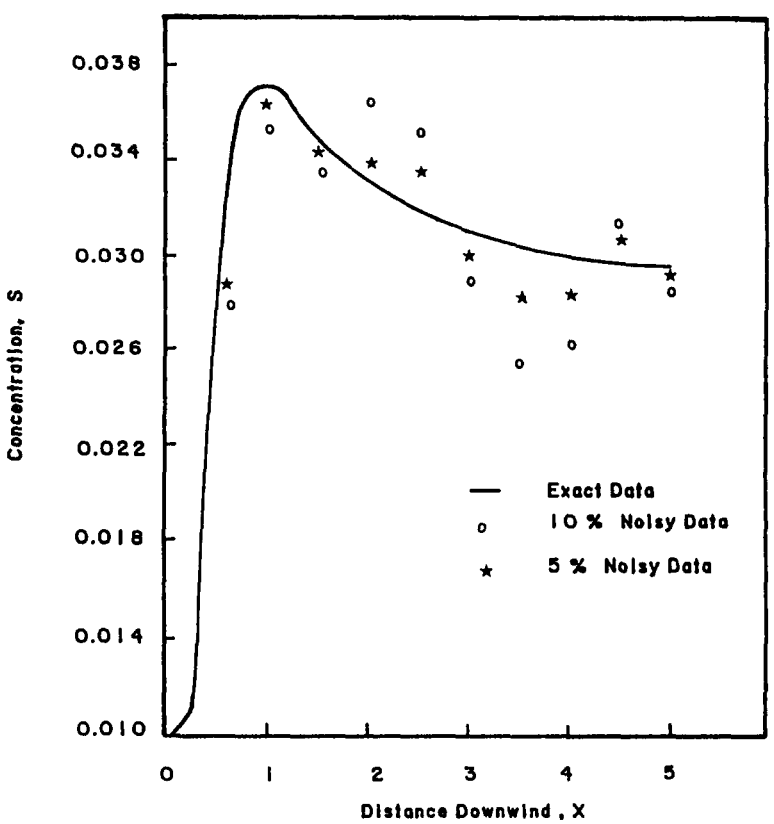

Figure 2. Actual and noisy measurements of SO_2 concentration in region $x5$.

To test the influence of initially assumed values for the five unknown parameters, the following 6 different sets of initial approximations were used.

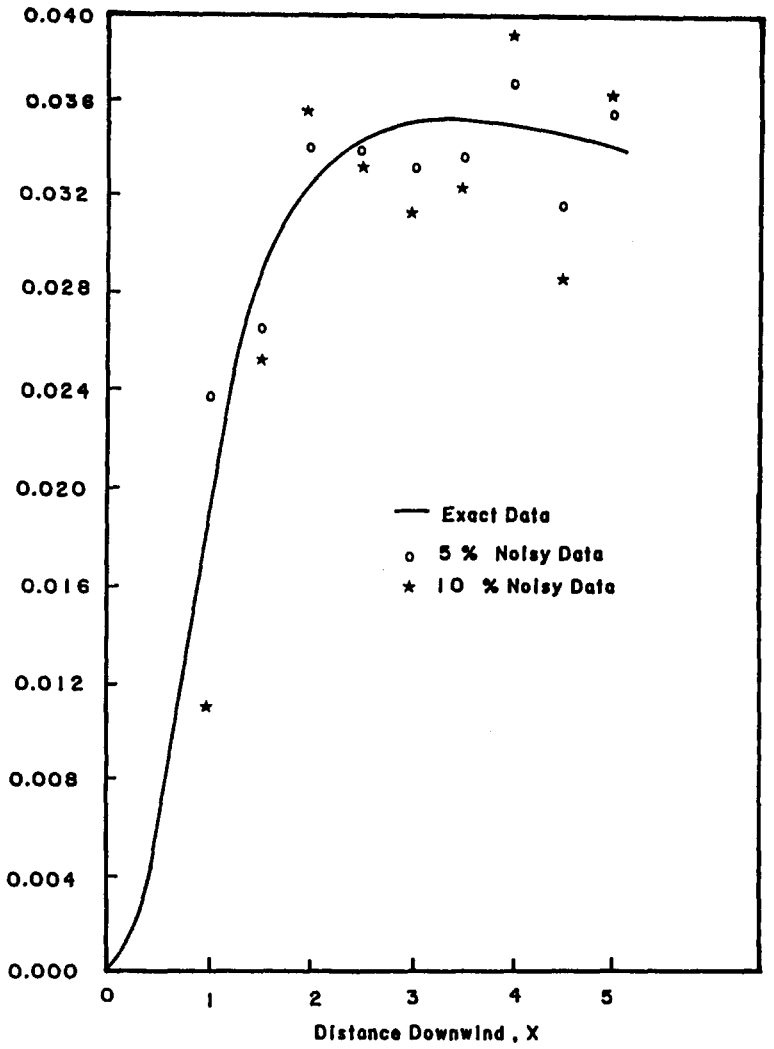

Figure 3. Actual and noisy measurements of SO_2 concentration in region $X6$.

(1) $V_{1,k=0}(X) = 4$, $V_{2,k=0}(X) = 2$, $V_{3,k=0}(X) = 0$, $V_{4,k=0}(X) = -1.5$, $V_{5,k=0}(X) = -3$,

(2) $V_{1,k=0}(X) = 6$, $V_{2,k=0}(X) = 4$, $V_{3,k=0}(X) = 0$, $V_{4,k=0}(X) = -3$, $V_{5,k=0}(X) = -5$,

(3) $V_{1,k=0}(X) = 10$, $V_{2,k=0}(X) = 6$, $V_{3,k=0}(X) = 0$, $V_{4,k=0}(X) = -5$, $V_{5,k=0}(X) = -8$,

(4) $V_{1,k=0}(X) = 15$, $V_{2,k=0}(X) = 10$, $V_{3,k=0}(X) = 0$, $V_{4,k=0}(X) = -5$, $V_{5,k=0}(X) = -10$,

(5) $V_{1,k=0}(X) = 20$, $V_{2,k=0}(X) = 15$, $V_{3,k=0}(X) = 0$, $V_{4,k=0}(X) = -10$, $V_{5,k=0}(X) = -15$,

(6) $V_{1,k=0}(X) = 50$, $V_{2,k=0}(X) = 45$, $V_{3,k=0}(X) = 0$, $V_{4,k=0}(X) = -30$, $V_{5,k=0}(X) = -35$.

for $0 \leq X \leq X_f = 5$. The computed data by solving equations (5)–(19) were used as the initial approximation functions for $x1, x2, \ldots, x15$ for all the calculations.

This problem was solved with the six different sets of initial approximations for the five unknown parameters. The convergence rates for all the six sets were very fast. The convergence rates for a typical set of initial approximations are shown in Tables 1 and 2 for the 5% and 10% noise level data, respectively. However, because only 11 experimental data points were used, the results are fairly far from the correct values, which are:

$$V_1 = 2.99, \quad V_2 = 1.35, \quad V_3 = 0, \quad V_4 = -1.11, \quad V_5 = -1.99.$$

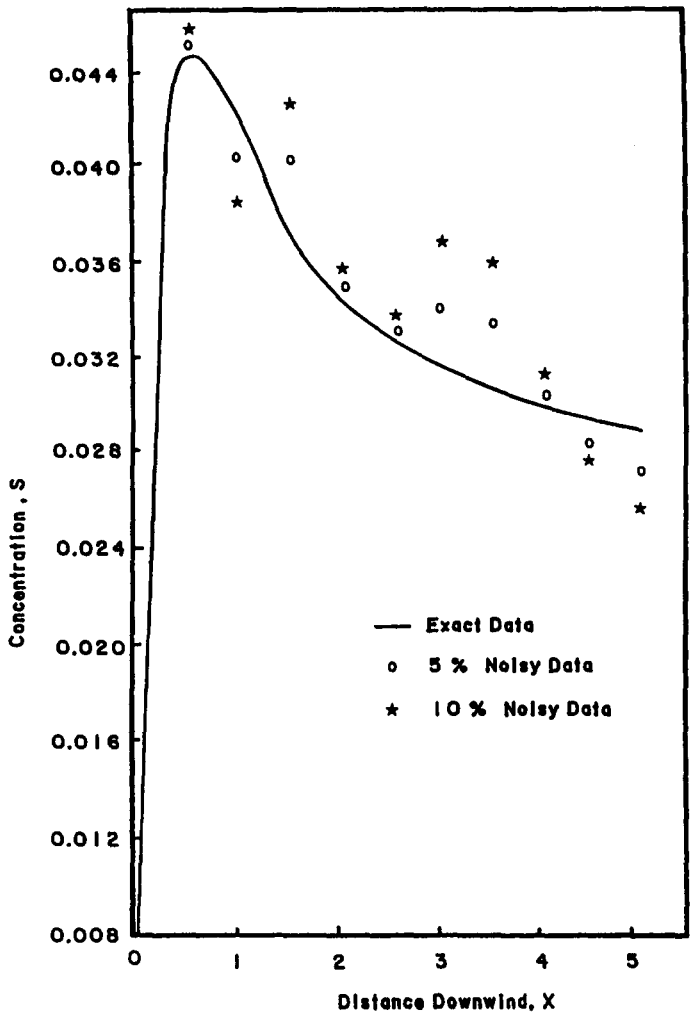

Figure 4. Actual and noisy measurements of SO_2 concentration in region $X13$.

If experimental data without any noise are used, with other numerical values remaining the same, the values obtained are very near the correct values as listed above for the V_s (see Tables 3 and 4).

Table 1. Convergence rates for V_1, V_2, V_3, V_4, and V_5 with 11 data points and 5% noise.

Iteration	V_1	V_2	V_3	V_4	V_5
0	6	4	0	-3	-5
1	2.7228	1.6857	-0.0690	-1.1877	-1.5817
2	2.6613	1.9111	-0.0713	-1.3678	-1.5496
3	2.6569	1.9144	-0.0690	-1.3865	-1.5283
4	2.6569	1.9144	-0.0686	-1.3884	-1.5258
5	2.6569	1.9144	-0.0686	-1.3887	-1.5255
6	2.6569	1.9144	-0.0686	-1.3887	-1.5255

To test further the influences of the number of experimental data on the estimated results, all 101 data points were first corrupted with 5% and 10% noise levels. The problem was again solved for all the six different sets by the quasilinearization procedure; some of the results are tabulated in Tables 5 and 6. The convergence rate is about the same as before. However, the

Table 2. Convergence rates for V_1, V_2, V_3, V_4, and V_5 with 11 Data Points and 10% noise.

Iteration	V_1	V_2	V_3	V_4	V_5
0	6	4	0	-3	-5
1	2.353	2.325	-0.114	-1.577	-1.006
2	2.279	2.505	-0.135	-1.706	-0.973
3	2.278	2.507	-0.131	-1.742	-0.929
4	2.278	2.507	-0.130	-1.750	-0.916
5	2.278	2.507	-0.130	-1.751	-0.916
6	2.278	2.507	-0.130	-1.751	-0.916

Table 3. Convergence rates for V_1, V_2, V_3, V_4, and V_5 with no noise and with initial approximation set 1.

Iteration	V_1	V_2	V_3	V_4	V_5
0	4	2	0	-1.5	-3
1	2.99951	1.35099	-0.00113	-1.10902	-1.99744
2	2.99998	1.35486	-0.00025	-1.11531	-1.99613
3	2.99996	1.35484	-0.00017	-1.11537	-1.99608
4	2.99996	1.35484	-0.00017	-1.11538	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 4. Convergence rates for V_1, V_2, V_3, V_4, and V_5 with no noise and with initial approximation data set 6.

Iteration	V_1	V_2	V_3	V_4	V_5
0	50	40	0	-30	-35
1	3.29695	1.09387	-0.00368	-0.863527	-2.25716
2	2.99873	1.35311	-0.00021	-1.11403	-1.99529
3	2.99999	1.35480	-0.00014	-1.11536	-1.99610
4	2.99996	1.35484	-0.00016	-1.11538	-1.99608
5	2.99996	1.35485	-0.00017	-1.11538	-1.99608
6	2.99996	1.35485	-0.00017	-1.11538	-1.99608

Table 5. Convergence rates for V_1, V_2, V_3, V_4, and V_5 with 101 data points and 5% noise.

Iteration	V_1	V_2	V_3	V_4	V_5
0	10	6	0	-5	-8
1	3.18333	1.23393	0.00414	-1.21487	-1.85879
2	3.18228	1.26013	0.00878	-1.24539	-1.82955
3	3.18257	1.25985	0.00924	-1.24602	-1.82933
4	3.18258	1.25983	0.00928	-1.24605	-1.82931
5	3.18258	1.28853	0.00929	-1.24605	-1.82931
6	3.18258	1.25983	0.00929	-1.24605	-1.82931

values estimated are nearer the true values. Futhermore, as expected, better values were obtained from data with lower noise levels.

Notice the fast convergence rates in spite of the very rough initial approximations. This is especially true if one compares Table 3 with Table 4. Thus, the quadratic convergence property, which is well known, shows clearly from these computations. This is one of the distinct advantages of quasilinearization.

Table 6. Convergence rates for V_1, V_2, V_3, V_4, and V_5 with 101 data points and 10% noise.

Iteration	V_1	V_2	V_3	V_4	V_5
0	10	6	0	-5	-8
1	3.37820	1.4119	0.01449	-1.37101	-1.70586
2	3.37276	1.15871	0.01998	-1.38363	-1.65298
3	3.37436	1.15741	0.02054	-1.38356	-1.65375
4	3.37446	1.15370	0.02059	-1.38356	-1.65378
5	3.37447	1.15729	0.02060	-1.38356	-1.65378
6	3.37447	1.15729	0.02060	-1.38356	-1.65378

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